# APPENDIX III

# DEVELOPMENT OF SITE SPECIFIC NUMERICAL STANDARDS FOR HUMAN AND ECOLOGICAL RECEPTORS

# APPENDIX IIIA

# TECHNICAL APPROACH

# Appendix IIIA
# Technical Approach

## 1.0 INTRODUCTION

An approach for developing site-specific numerical standards (SSNS) was developed for VPH and LEPH. The approach is consistent with guidance issued by Yukon Renewable Resources, which recommended as one option the application of the CCME (1996a) method. The Canadian Council of Ministers of the Environment (CCME, 1996a) endorses the use of a risk-based approach, which has been applied here to determine levels in soil that would be sufficiently low to protect receptors potentially exposed to volatile contaminants associated with the VPH and LEPH fractions. The following sections discuss:

- receptors, contaminants of concern, and exposure pathways,
- selection of appropriate surrogates for VPH and LEPH,
- receptor and exposure assumptions,
- method for modelling air concentrations, and
- approach used to calculate acceptable levels of VPH and LEPH in soil.

## 2.0 PROBLEM FORMULATION

### 2.1 Site Description

The site is in semi-arid climate and is sandy with large open areas. Trees and other vegetation are present on approximately 30% of the site. The land use is classified as commercial/industrial, but the site is vacant and fenced and there are no plans for future activities. The hydrocarbon contamination, which was found on approximately 10% of the site, has been excavated to a depth of 3 m.

### 2.2 Receptors

The potential receptors on-site include human and terrestrial ecological receptors. Since the site will remain vacant, the only potential human receptor is a trespasser visiting the site for short periods of time. Ground squirrels were observed on the site and other small mammals and birds could be present. Because the contamination is restricted to depths of greater than 3 m, plants and soil invertebrates would not be potential receptors.

Aquatic receptors were not considered as potential receptors since the PAH concentrations in recently monitored wells were below applicable standards at the site, and iron and manganese exceedances are most likely related to regional groundwater quality (Golder, 1998). Furthermore, the groundwater travel time from the site to Bennett

Lake is estimated to be on the order of 100 years and natural attenuation would retard the rate of contaminant migration. No evidence of petroleum contamination was detected in a well located between the site and Bennett Lake.

### 2.3 Contaminants of Concern

Based on the chemical data collected at the site, the only contaminants of concern (COCs) are hydrocarbons associated with the VPH and LEPH fractions. Concentrations of VPH, constituents of VPH including toluene and xylene, and LEPH were elevated (i.e., greater than Yukon CSR Industrial Land Use standards) in soil samples collected at depths of 3 m or more.

### 2.4 Exposure Pathways and Conceptual Exposure Model

The soil contamination is restricted to depths of greater than 3 m, making direct contact with the contamination insignificant for all receptors. Human and terrestrial ecological receptors could be exposed to volatile contaminants via inhalation. A conceptual exposure model was prepared summarizing the potentially significant exposure pathways (Figure IV-1).

## 3.0 DEVELOPMENT OF SITE SPECIFIC NUMERICAL STANDARDS

### 3.1 Selection of Surrogate Compounds for Petroleum Hydrocarbon Fractions

Assessing the toxicity of individual hydrocarbons is difficult if not impossible due to excessive analytical and computational requirements, and insufficient data for many hydrocarbons. To overcome this problem, many of the new approaches involve delineating total petroleum hydrocarbons into fractions determined based on the physical and chemical properties of the hydrocarbons in a particular carbon range (TPHCWG, 1997; Commonwealth of Massachusetts, 1997). Surrogate hydrocarbons are then selected to represent each chemical class within each fraction (*e.g.*, aliphatic or aromatic hydrocarbons), based on their physical, chemical, and toxicological properties. This results in fraction-specific toxicity values for non-carcinogenic hydrocarbons (carcinogenic hydrocarbons such as benzene are typically assessed on an individual basis).

In 1995, Golder prepared a document for BC Environment (BCE) entitled, *Recommendations to BC Environment for Development of Remediation Criteria for Petroleum Hydrocarbons in Soil and Groundwater*. For the current assessment the BCE approach was adopted. CCME has developed an integrated approach to dealing with total petroleum hydrocarbon contamination in the soil but the approach is in draft form, CWS-PHC Draft June 2000.

The fundamental characteristics of the approach used to deriving remediation criteria for petroleum hydrocarbons are listed below:

1. Surrogates are chosen to represent non-carcinogenic chemicals in petroleum hydrocarbons. Analysis for specific carcinogenic chemicals will be conducted when warranted.
2. Petroleum hydrocarbons are quantified for the following three carbon boiling ranges:
   - Volatile petroleum hydrocarbons (VPH): n-$C_5$ to n-$C_9$
   - Light extractable petroleum hydrocarbons (LEPH): n-$C_{10}$ to n-$C_{18}$
   - Heavy extractable petroleum hydrocarbons (HEPH): n-$C_{19}$ to n-$C_{32}$
3. Within each boiling range fraction, surrogates are chosen to represent two chemical classes: alkanes/cylcloalkanes and aromatics/alkanes.

At the site, the contamination appears to consist primarily of diesel-related hydrocarbons. Diesel is a middle distillate fuel with the majority of their hydrocarbon compounds in the $C_{10}$ to $C_{18}$ range. This fuel can be classified into three fractions, VPH, LEPH, and HEPH, according to the framework outlined above. The HEPH fraction can be generally characterized as non-volatile, non-soluble and non-mobile, and is likely to remain at the release site (TPHCWG, 1997). LEPH is more mobile and volatile than HEPH and VPH is the lightest, most volatile and mobile fraction. Fresh diesel consists of approximately 17% VPH, 71% LEPH, and 12% HEPH (K. Thomas, Analytical Services Laboratory, pers.com., 1998). For diesel fuel, inhalation of VPH along with potentially volatile contaminants in the LEPH range could be of concern at this site.

Surrogates for VPH and LEPH were selected and evaluated in the risk assessment. Documents published by the Total Petroleum Hydrocarbon Criteria Working Group Series (TPHCWG, 1997) and Golder (1995) were consulted for information on applicable surrogates for each fraction. Surrogates were chosen separately for the volatile aromatic and aliphatic fractions of VPH and LEPH as the toxicity of these two fractions is significantly different.

Golder (1995) estimated that VPH is made up of 40% aromatics and 60% aliphatics. The toxicity of VPH can be evaluated by using toluene as a surrogate for the aromatic fraction and hexane as a surrogate for the aliphatic fraction (refer to Table 1).

Although the volatility of most hydrocarbons in the LEPH range is low, a conservative screening approach was taken in the current assessment and 100% of LEPH was assumed to be volatile. If the results under this approach indicate levels at the site are acceptable, a more detailed, realistic analysis is not required. The surrogate for the volatile aromatic fraction of LEPH is naphthalene, the most toxic aromatic contaminant in the $C_{10}$-$C_{18}$ range (Golder, 1995). The surrogate for the volatile aliphatic portion of LEPH is decane

(Golder, 1995). Golder (1995) estimated that aliphatic compounds represent 80% of the LEPH fraction, and aromatic compounds the remaining 20%.

**Table 1**
**Surrogate Compounds Used in Derivation of SSNS**

| Fraction | Surrogate | % of VPH or LEPH Fraction |
|---|---|---|
| VPH - Aliphatic | Hexane | 60% |
| VPH - Aromatic | Toluene | 40% |
| LEPH - Aliphatic | Decane | 80% |
| LEPH – Aromatic | Naphthalene | 20% |

## 3.2 Calculation of SSNS for Human Receptors

To calculate the SSNS for the petroleum hydrocarbon fractions, a series of steps are required. The toxicity of the surrogate compounds representing the hydrocarbon fractions must be evaluated, and represented by a guidance value. The site-specific assumptions regarding receptor exposure must be established. The toxicity information is then combined with the exposure assumptions to determine the level of petroleum hydrocarbon in soil that would be acceptable. Because the exposure pathway of interest at the site is inhalation of volatiles, the acceptable level petroleum hydrocarbons of soil is based on the predicted acceptable vapour flux to outdoor air. The steps in deriving the SSNS are described in the following sections.

### 3.2.1 Toxicity Assessment for Surrogates

Health Canada classifies contaminants based on their mode of action (*i.e.*, threshold vs. non-threshold substances). For substances exhibiting a *threshold* for toxicity, an acceptable level of exposure below which no adverse effects are anticipated is established. This level is referred to as a tolerable daily intake (TDI) or reference dose (RfD). For *non-threshold* chemicals (*e.g.*, some carcinogens), any level of exposure is assumed to pose a potential risk. A slope factor, which expresses the cancer risk per unit dose, is derived for carcinogens and used to predict risks at the observed exposures.

The four surrogate compounds (naphthalene, decane, hexane and toluene) are considered non-carcinogens. Reference doses (RfDs) were determined for each of the surrogate compounds based on literature sources. The RfDs are summarized in the Table 2 and further information regarding the derivation of RfDs is provided in Appendix 1B.

**Table 2**
**Reference Doses for Surrogate Contaminants for the Human Receptor**

| Chemical | Inhalation RfD* (mg/kg-d) | Reference |
|---|---|---|
| Hexane | $6.57 \times 10^{-2}$ | U.S. EPA (1999) |
| Toluene | 1.25 | Health Canada (1996) |
| Decane | 1.02 | SCS (1994) |
| Naphthalene | $9.86 \times 10^{-4}$ or $1.6 \times 10^{-2}$ | U.S. EPA (1999); Health Canada (1992) |

* Certain values were converted from mg/$m^3$ to mg/kg-d using a breathing rate of 6 $m^3$/day and body weight of 70.7 kg (CCMEb, 1996).

### 3.2.2 Receptor and Exposure Assumptions

A teenage trespasser (aged 12 to 19) was assumed to be on-site for 1 hour per day, 365 days per year. Table 3 summarizes the relevant exposure parameters for the receptor.

**Table 3**
**Exposure Parameters**

| Parameter | Value |
|---|---|
| Respiration Rate Teenager | 0.875 $m^3$/hr |
| Body Weight Teenager | 57 kg |
| Exposure Frequency | 365 d/yr |
| Exposure Duration | 8 yr (from age 12 through age 19) |
| Daily Exposure (inhalation) | 1 hr/d |
| Averaging Time Non-carcinogens | 8 yr |

4. Note: All exposure parameters used are based on the typical average values for the Canadian population and were taken from CCME (1996b).

### 3.2.3 Modelling of Outdoor Air Concentrations

The results of the environmental assessment for the site indicate that there are two main areas of soil contamination at the site. The LEPH contamination encompasses a total area of approximately 1700 $m^2$ and is located at a depth of 3.0 m. The VPH contamination encompasses an area of approximately 1200 $m^2$ and is also located at a depth of 3.0 m. Since the LEPH and VPH contamination is located at depth, the only exposure pathway for humans is via inhalation of volatile compounds in outdoor air. A soil gas model was used to estimate exposure from this pathway, as discussed below.

A quasi-analytical spreadsheet model was used to predict exposure concentrations in air based on soil concentrations. Two exposure scenarios were considered:

1. Volatilization of LEPH (represented by naphthalene and decane) from subsurface soils into outdoor air, where a teenage trespasser could be exposed via inhalation.
2. Volatilization of VPH (represented by toluene and hexane) from subsurface soils into outdoor air, where a teenage trespasser could be exposed via inhalation.

The following environmental fate and transport mechanisms were modelled: 1) chemical partitioning between soil and soil gas, 2) migration of vapour through soils due to diffusion, 3) dilution of airborne chemicals through wind-driven airflow. It was assumed that the contaminated soil was present at 3 m depth and covered with clean soil, based on the field investigation results. The outdoor soil gas model is described in detail in Appendix 1C.

### 3.2.4 Calculation of Site-Specific Numerical Standards

To determine the acceptable level of VPH and LEPH in soil, a series of calculations was carried out as discussed below.

1. The initial concentrations of VPH and LEPH in soil were set at 1 mg/kg. The concentrations of the surrogate compounds were assumed to be as follows: toluene (0.4 mg/kg), hexane (0.6 mg/kg), naphthalene (0.2 mg/kg) and decane (0.8 mg/kg), based on the relative fractions of volatile aliphatic and aromatic constituents (see Section 3.1). The starting soil concentrations for the surrogates are arbitrary, with the only condition being that they are below the soil saturation limits (discussed in more detail below).
2. The soil gas model was run using the soil concentrations from step 1 and hazard quotients (HQs) for each surrogate calculated.
3. Based on the results of step 3, the soil concentration for each surrogate corresponding to a target hazard quotient of 1 was determined using a simple back calculation that assumed linear increase in risk with increase in soil concentration. This is the typical approach applied in noncancer risk assessment and in most cases these results would be used to set acceptable levels in soil. However, because at the current site the chemicals of concern are volatile and the pathway of interest is inhalation, the behaviour of the volatile chemical found in soil must be considered in setting the acceptable soil level (step 5).
4. The acceptable soil concentrations determined in step 4 were compared to the soil saturation limits for each surrogate, as predicted by the model. The soil saturation limit corresponds to the soil concentration at which no nonaqueous phase liquid is present. Above the soil saturation limit, the predicted soil vapour level of the contaminant remains constant and thus the resultant risks also remain constant. Thus,

if the HQ is below 1 at the soil saturation limit, the HQ would be below 1 at any contaminant soil concentration. If the acceptable soil concentration of the surrogate predicted in step 4 using a simple back calculation is below the corresponding soil saturation limit, then an acceptable LEPH or VPH soil concentration could be determined. If the acceptable soil concentration of the surrogate is above the soil saturation limit, the risks from inhalation exposure would be acceptable at any soil concentration and an upper limit acceptable soil concentration for LEPH or VPH cannot be determined (i.e., risks are acceptable regardless of the concentration).

5. Depending on the outcome of step 5, an acceptable VPH and LEPH concentration would be generated based on the modelling results for the surrogates.

Relevant equations are summarized below.

Calculation of Dose Rates for Surrogates

$$DR_{surrogate} = \frac{IR \times ET \times C_{air\ surrogate} \times EF \times ED \times BF}{BW \times AT \times CF}$$

Calculation of Hazard Quotients for Surrogates

$$HQ_{surrogate} = DR_{surrogate}/RfD_{surrogate}$$

Calculation of Soil Concentration Corresponding to a Target Hazard Quotient of 1

$$C_{acceptable} = C_{initial} \times THQ/HQ_{surrogate}$$

where:

$DR_{surrogate}$ = dose rate via inhalation of volatiles (mg/kg-d);
IR = inhalation rate ($m^3$/hr);
ET = exposure time (hr/d);
$C_{air\text{-}surrogate}$ = modelled concentration of volatile in air (mg/$m^3$);
EF = exposure frequency (d/yr);
ED = exposure duration (yr);
BW = body weight (kg);
AT = averaging time (yr);
CF = unit conversion factor to convert years to days, 365 d/yr;
BF = bioavailability factor for inhalation (equal to 1).
$HQ_{surrogate}$ = Hazard quotient for surrogate compound (unitless)
$RfD_{surrogate}$ = Reference dose for surrogate compound (mg/kg-d)
$C_{acceptable}$ = Soil concentration of surrogate corresponding to target hazard quotient of 1 (mg/kg)
$C_{initial}$ = Initial soil concentration of surrogate (mg/kg) (arbitrary; based on VPH and LEPH soil concentrations of 1 mg/kg)
THQ = Target hazard quotient (1; unitless)

The modelling results showed that for all surrogates of VPH and LEPH, the soil saturation limits for the surrogates are associated with HQs of less than 1. Once the soil saturation level is reached, risks remain constant even with increasing levels of chemical being added to the soil. This means that an upper limit safe level cannot be calculated and regardless of VPH and LEPH concentrations in soil risks are acceptable.

### 3.3 Calculation of SSNS for Ecological Receptors

Inhalation pathways are generally not quantified for ecological receptors. However, because that pathway is the only relevant one at this site, exposure to volatile contaminants in outdoor air was quantified for the mouse using the same procedure described for human receptors above. A white-footed mouse (*Peromyscus leucopus*) was used to estimate risk to potential mammalian ecological receptors at the Carcross tank farm. The white-footed mouse inhabits a small territory and was assumed to live in the area of concern at the site everyday for 24 hr/d. The body weight for a white-footed mouse was assumed to be 0.022 kg (Green and Miller, 1987) and the inhalation rate was calculated to be 0.032 $m^3/d$ based on an allometric equation published by the US Environmental Protection Agency (Anderson et al., 1983). Toxicity reference values relevant to the mouse are reported in Appendix IVB.

The results indicated that the hazard quotients were less than 1 at the soil saturation limit. Therefore, an upper limit acceptable soil concentration cannot be established for the exposure scenario of a mouse inhaling vapours in outdoor air.

### 3.4 Summary of Results

The soil saturation limits are as follows for the surrogates (rounded to two significant figures): 1000 mg/kg for toluene, 280 mg/kg for hexane, 250 mg/kg for naphthalene, and 62 for decane. The maximum hazard quotients associated with these soil saturation limits are shown in the following table for the human and ecological receptors:

| **Surrogate** | **Soil Saturation Limit[a] (SSL)** | **Hazard Quotient for Human Receptor at SSL** | **Hazard Quotient for Ecological Receptor at SSL** |
|---|---|---|---|
| | **mg/kg** | **(unitless)** | **(unitless)** |
| Toluene | 1000 | 0.00088 | 0.0040 |
| Hexane | **280** | 0.10 | 0.012 |
| Naphthalene | 250 | 0.0037[b]<br>0.0060[b] | 0.0000042 |
| Decane | 62 | 0.00010 | 0.000045 |

[a] Predicted by soil gas model and rounded to two significant figures (see Appendix IVC for more details).

[b] The two hazard quotients reported for naphthalene are based on the two available reference doses for naphthalene (described in Appendix IVB).

The HQ's at the soil saturation limit are at least an order of magnitude less than 1; therefore, the soil saturation limit is acceptable.

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# APPENDIX IIIB

# CHEMICAL-SPECIFIC TOXICITY DATA

# Appendix IIIB
# Chemical-Specific Toxicity Data

The following sections describe the available toxicity reference values for the surrogate chemicals in the alkane and aromatic fractions of volatile petroleum hydrocarbons (VPH) and light extractable petroleum hydrocarbons (LEPH). Section 1 provides the human toxicity data and Section 2 discusses the data for ecological receptors.

## 1.0 TOXICITY DATA FOR HUMAN RECEPTORS

### 1.1 Decane

A NOAEL of 540 ppm was determined for decane by SCS (1994) based on a subchronic inhalation study on rats exposed to decane in air for 17 hours per day over 91 days. Although no statistically significant effects were noted in this study, the authors observed that mean body weights of treated animals were increased compared to controls and the mean white blood cell count (WBC) in the treatment group was decreased at 57 days after treatment and increased at 91 days after treatment in comp arison to the mean WBC for the controls. The NOAEL of 540 ppm was converted to a concentration in air of 3,142.8 mg/m$^3$. An uncertainty factor of 1000 (10 each for interspecies and intraspecies variability, and 10 for extrapolation from a subchronic to chronic NOAEL) was applied to end up with an RfC of 3.1 mg/m$^3$. The RfC was converted to a RfD of 1.0 mg/kg-d by assuming an inhalation rate of 23 m$^3$/d and a body weight of 70 kg (CCME, 1996).

### 1.2 Hexane

The US EPA (1999) has reported an inhalation RfC of 0.2 mg/m$^3$ for n-hexane, based on an epidemiological inhalation study in humans and is supported by a subchronic study in mice. This RfC was converted to 0.066 mg/kg-d assuming an inhalation rate of 23 m$^3$/d and a body weight of 70 kg (CCME, 1996). The LOAEL identified in the human epidemiological study was 204 mg/m$^3$ (58 ppm) and was adjusted to 73 mg/m$^3$ to account for exposure duration. The reported effects at the LOAEL were neurotoxicity and electrophysiological alterations. An uncertainty factor of 300 was applied to the adjusted LOAEL of 73 mg/m$^3$ to account for intraspecies variability (10), use of a LOAEL rather than a NOAEL (10) and a lack of data for reproductive and chronic effects (3), resulting in an RfC of 0.2 mg/m$^3$ (or 0.066 mg/kg-d).

### 1.3 Naphthalene

An inhalation RfC of 0.003 mg/m$^3$ was established for naphthalene by the US EPA (1999) based on a chronic study in which mice were exposed to naphthalene in the air 6 hours per day, 5 days per week for 103 weeks. A LOAEL of 9.3 mg/m$^3$ was identified, based on nasal effects that included hyperplasia and metaplasia in respiratory and olfactory epithelium. Application of a safety factor of 3,000 (10 each for interspecies and intraspecies variability, and 10 for extrapolation from a LOAEL to a NOAEL and 3 for database deficiencies) was used for derivation of an RfC. The RfC was converted to a RfD of $9.86 \times 10^{-4}$ mg/kg-d by assuming an inhalation rate of 23 $m^3$/d and a body weight of 70 kg.

The Chemical Health Hazard Assessment Division in the Food Directorate of Health Canada has evaluated naphthalene. Naphthalene has long been used as a household fumigant against clothes moths but has no food use in Canada. A provisional TDI (pTDI) of 0.016 mg/kg-d was derived by Health Canada in 1992 (M. Cheng, Health Canada, pers comm, 1998). A LOAEL of 16 mg/kg-d for cataract formation was identified in a rabbit study. A safety factor of 1000 was applied to the LOAEL to produce the pTDI.

The soil gas model was run using both the Health Canada pTDI of 0.016 mg/kg-d and the inhalation RfD of $9.86 \times 10^{-4}$ mg/kg-d based on US. EPA (1999).

### 1.4 Toluene

Toluene is treated as a noncarcinogen in Canada. An inhalation tolerable daily intake for toluene of 1.25 mg/kg-d based on an animal study was derived under CEPA (1992). The TDI was based on a bioassay that detected a decreased body weight in mice exposed to toluene. The LOAEL of 375 mg/$m^3$ was converted to a RfD using conversion factors for mice and an uncertainty factor of 100, to account for intraspecies variation and extrapolation from animals to humans ((375 mg/$m^3$ x 0.043 $m^3$/d x 6.5/24 x 5/7)/(0.025 kg x 100)). No safety factor was included to account for the difference between a LOAEL and NOAEL, because the observed effect was a decrease in body weight without other evidence of toxicity. Additionally, no factor was included to account for the fact the key study was less than a chronic bioassay because NOAELs observed in other chronic studies were higher than the LOAEL used here. A RfC of 3.8 mg/$m^3$ was derived based on studies in humans and reported in Health Canada (1996). Applying the breathing rate of 23 $m^3$/d and 70 kg recommended by BCE (1996) and CCME (1996) for an adult gives a RfD of 1.25 mg/kg-d. Based either on the animal or human studies, the estimated inhalation RfD for toluene is 1.25 mg/kg-d.

## 2.0 TOXICITY DATA FOR ECOLOGICAL RECEPTORS

### 2.1 Decane

A NOAEL of 540 ppm was reported for rats exposed to decane vapour for 18 hr/d, 7 d/wk for a total of 123 days (Nau et al., 1966). The NOAEL was converted to 3142 mg/$m^3$ (540 ppm x 142.3 g/mol / 24.45 L/mol assuming 25C). The value of

3142 mg/m$^3$ was converted to 2160 mg/kg-d using data for Sprague-Dawley rats from EPA (1988) for inhalation rate and body weight ((3142 mg/m3 x 0.22 m$^3$/d x [18hr/d/24hr/d] x 123d)/(0.240kg bw x 123 d)). An uncertainty factor of 10 was applied to derive a TRV of 216 mg/kg-d.

## 2.2 Hexane

A NOAEL of 1762 mg/m$^3$ and LOAEL of 3525 mg/m$^3$ were reported in a 90-d mouse inhalation study with hexane (Dunnick et al., 1989). The US EPA (1999) converted the NOAEL and LOAEL concentrations to 315 mg/m$^3$ and 629 mg/m$^3$, respectively, since the mice were exposed to hexane 6 hr/d for 5 d/wk. The LOAEL was based on epithelial lesions in the nasal cavity of mice. No oral studies on which to base an oral TRV were identified in the literature reviewed. As a result, the NOAEL from the inhalation study of 315 mg/m$^3$ was converted to 528 mg/kg-d for mice assuming an inhalation rate of 0.053 m$^3$/d and weight of 0.0316 kg (EPA, 1988). An uncertainty value of 10 was applied to derive a TRV of 52.8 mg/kg-d.

## 2.3 Naphthalene

No observed adverse effects were reported in a subchronic study in which laboratory mice were orally exposed to a naphthalene concentration of 133 mg/kg-d (Shopp et al., 1984). The subchronic oral toxicity of naphthalene was evaluated using CD-1 mice in a 90-day gavage study (Shopp et al., 1984). The mice received doses of 5.3, 53, or 133 mg/kg-d. The authors reported no adverse effects on body weight or treatment-related mortality at any level. High-dose females were reported to have decreased brain, liver, and spleen weight, and there was a decreased spleen weight to body weight ratio. Shopp et al. (1984) reported no significant effects on the immune system at any dose. The NOAEL of 133 mg/kg-d from the 90-day laboratory mouse study was adopted as the TRV.

## 2.4 Toluene

Sample et al. (1996) derived a NOAEL of 26 mg/kg-d for white-footed mice exposed to toluene. This was based on a teratogenicity study in mice administered toluene via oral gavage at 0.3, 0.5 or 1.0 mL/kg/d during days 6 to 12 of gestation. Reduced fetal weight was reported for the two highest dose groups and embryomortality was reported to be significantly reduced for all dose groups. A LOAEL of 260 mg/kg-d was reported, despite the fact that this value was calculated from the lowest dose group. Sample et al. (1996) calculated a NOAEL of 26 mg/kg-d using an uncertainty factor of 10. The calculation of the NOAEL was justified since the study took place during a critical lifestage. The NOAEL of 26 mg/kg-d was adopted as the TRV.

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# APPENDIX IIIC

# SOIL VAPOUR MODEL

# Appendix IIIC
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## 1.0 GENERAL

This appendix provides a generic description of the outdoor soil gas infiltration model developed by Golder. For the purposes of this assessment, toluene and hexane were used as surrogates for the aromatic and aliphatic constituents of the measured VPH fraction and naphthalene and decane were used as surrogates for the aromatic and aliphatic constituents of the measured LEPH fraction. The outdoor soil gas model was used to model the infiltration of vapours to outdoor air.

The model calculations consist of two main components: (1) estimation of environmental fate and transport rate for volatiles in soil gas and resulting outdoor air exposure concentrations and (2) estimation of risks based on the exposure concentrations. The model used to predict the soil gas transport is a semi-analytical deterministic spreadsheet model. The model is relatively simple and can be used in situations when the type and amount of data is limited. The overall level of conservatism is considered appropriate for a screening-level model.

## 2.0 DESCRIPTION OF MODEL

The soil gas infiltration and exposure model calculates risk levels for transport of individual volatile chemicals in soil gas into outdoor air, inhalation exposure rates, and specified soil and groundwater concentrations. The model includes the following key components:

1. Partitioning between soil (adsorbed), soil-water and soil-air (three phase system) or between NAPL, soil (absorbed), soil-water and soil-air (four phase system);
2. Steady-state one-dimensional diffusion through soil-air; and
3. Steady-state dilution in outdoor air through wind-driven airflow.

The soil gas model consists of diffusion through a two-layer system, and incorporates dilution provided by wind-driven air flow. The two-layers can either be two different soil types, or soil and a concrete or asphalt surface slab. Physical-chemical parameters used for the risk assessment modelling are presented in the table presented below.

| Chemical | MW (g/mol) | Vapour Pressure @ 20-25°C (atm) | Henry's Law Coefficient (atm $m^3$/mol) | Solubility @ 20-25°C (mg/L) | Partition Coefficient Log Koc ($cm^3$/g) | Octanol/water Partition Coefficient Log Kow ($cm^3$/g) | Air Diffusivity Coef. M (slope) ($m^2$/sec) | Air Diffusivity Coef. B (intercept) ($m^2$/sec) |
|---|---|---|---|---|---|---|---|---|
| Hexane | 86 | 1.99E-01 | 1.7 | 9.5 | 3.53 | 4.11 | 4.60E-08 | 6.56E-06 |
| Toluene | 92 | 3.75E-01 | 6.74E-03 | 515 | 2.48 | 2.73 | 4.80E-08 | 6.88E-06 |
| Decane | 142 | 1.7E-03 | 6.91 | 0.052 | 5.29 | 6.25 | 3.6E-08 | 5.1E-06 |
| Naphthalene | 128 | 7.2E-04 | 6.2E-04 | 32 | 3.11 | 3.31 | 3.9E-08 | 5.6E-06 |

The components of the model are further described below.

## 3.0 PARTITIONING

Equilibrium partitioning is assumed between chemicals in the sorbed, soil-water and soil-air phases (three phase system) with no non-aqueous phase liquids (NAPL) present in soil or between NAPL and above three phases (four phase system). To determine which model is appropriate for use, the soil saturation concentration ($C_{sat}$) (i.e., concentration above which NAPL is present) is estimated for individual chemicals using the equation presented in Exhibit 1. The soil saturation concentration is estimated using a revised equation described in a memorandum from J. Dinan of the U.S. EPA to Regional Toxic Integration Coordinators (date-stamped November 9, 1992), except modified to include provision for mole fraction of chemical in multi-component mixture. The equilibrium partitioning model used is the Freunlich isotherm assuming linear partitioning.

**Exhibit 1 - Determination of Soil Saturation Concentration for a Given Chemical**

$$C_{sat} = X \times \frac{S}{\beta} (K_d \times \beta + P_w + H' \times P_a)$$

where:

| Parameter | Definition (units) | Default |
|---|---|---|
| $C_{sat}$ | Soil saturation concentration (mg/kg) | |
| $K_d$ | Soil-water partition coefficient (mg/kg-soil per mg/L-water) | Chemical-specific, or $K_{oc} \times f_{oc}$ |
| $K_{oc}$ | Organic carbon partition coefficient (mg/kg-OC per mg/L-water) | Chemical-specific |
| $f_{oc}$ | Organic carbon content of soil (kg-OC/kg-soil) | Site-specific, or 0.006 kg/kg |
| S | Solubility in water (mg/L-water) | Chemical-specific |
| $\beta$ | Soil dry bulk density (kg-soil/L-soil) | 1.6 kg/L |
| $P_w$ | Water-filled soil porosity (unitless) | $P_t - P_a$ |
| H' | Henry's Law constant (unitless) | H × 42.3, where 42.3 is a units conversion factor @ 15°C |
| H | Henry's Law constant (atm-$m^3$/mol) | Chemical-specific |
| $P_a$ | Air-filled soil porosity (unitless) | $P_t - \theta = 0.2$ |
| $\theta$ | Average unsaturated zone soil volumetric water content (L-water/L-soil) | $\theta_m \beta / \rho_w = 0.2$ |
| $\theta_m$ | Average unsaturated zone soil gravimetric water content (kg-water/kg-soil) | 0.12 |
| $\rho_w$ | Density of water (kg-water/L-water) | 1 kg/L |
| $P_t$ | Total soil porosity (unitless) | $1 - \beta/\rho_s = 0.4$ |
| $\rho_s$ | True soil density or particle density (kg-soil/L-soil) | 2.65 kg/L |
| X | mole fraction of chemical in contaminant mixture | Chemical specific |

**Exhibit 2 - Phase Partitioning**

If $C_t < C_{sat}$ then

$$C_{sw} = \frac{C_t \times \beta}{(K_{oc} \times f_{oc} \times \beta + Pw)} \quad \text{Eq. 1}$$

$$C_{sg} = 1000 \times C_{sw} \times H' \quad \text{Eq. 2}$$

Else

$$C_{sw} = X \times S \quad \text{Eq. 1b}$$

$$Csg = \frac{1E06 \times X \times P \times MW}{R \times T} \quad \text{Eq. 2b}$$

| Parameter | Definition (units) | Default |
|---|---|---|
| $C_t$ | Total contaminant concentration in soil (mg/kg) | -- |
| Csw | Contaminant concentration in soil water (mg/L) | -- |
| Csg | Contaminant concentration in soil gas (mg/m$^3$) | -- |
| $K_{oc}$ | Organic carbon partition coefficient (mg/kg-OC per mg/L-water) | Chemical-specific |
| $f_{oc}$ | Organic carbon content of soil (kg-OC/kg-soil) | 0.006 |
| H′ | Henry's constant (unitless - conversion factor of 42.3 based on 15 deg C) | Chemical-specific |
| H | Henry's constant (atm-m$^3$/mol) | Chemical-specific |
| P | Pure-phase vapour pressure of chemical (atm) | Chemical-specific |
| MW | Molecular weight (g/mole) | Chemical-specific |
| R | Universal gas constant (L-atm / K-mole) | 0.08205 |
| T | Temperature (°K) | 288 |

Since petroleum hydrocarbons consist of a mixture of chemicals, the actual soil saturation concentration will depend on the properties of the mixture and will be lower than for a pure-chemical due to the affects of co-solubility. In soil where NAPL is present, the soil gas concentration for a particular chemical will be directly related to the partial pressure of the chemical in the mixture and the molecular weight. Furthermore, the soil gas concentration will be independent on the concentration of the chemical in soil (*i.e.* constant).

The soil gas concentrations predicted using the non-NAPL partitioning equations (Exhibit 2) will be conservative and exceed soil gas concentrations predicted using equilibrium phase transfer models assuming NAPL is present. Therefore, use of linear partitioning is considered to be justified for derivation of generic criteria where no specific information on product composition is available.

The partitioning model assumes that sufficient soil moisture is present to form at least a monolayer water film over soil particulates. Batterman et. al. (1995) suggests that "dry" soils with less than a monolayer water film will have soil moisture contents less than 2 percent. For "dry" soils, partitioning will occur between the absorbed and soil-gas phase and therefore, the partitioning model used may not be valid for soils that are in a "dry" state (e.g., volcanic tuff deposits). The Brauner-Emmett-Tellar (BET) equation can be used to estimate the equilibrium vapour pressure of chemicals sorbed to dry soil (Valsaraj and Thibodeaux, 1988).

The contamination source is assumed to be infinite in lateral extent but vertically depletable for the soil to air transport pathway (but not for the groundwater to air transport pathway). Source depletion is incorporated using a mass-balance approach and is bounded by the vertical extent of contamination, the source is assumed to be entirely depleted (i.e., soil gas concentrations are set to zero).

## 4.0 CONTAMINANT FATE AND TRANSPORT

Soil gas fate and transport is based on one-dimensional upward diffusion through air in soil and concrete/topsoil with no attenuation due to biodegradation (i.e., Farmer model). The model incorporates both diffusion through intact concrete and cracks in a concrete or asphalt slab or topsoil. A single, homogenous soil layer and steady-state transport (i.e., no retardation) is assumed. The mathematical equations for contaminant fate and transport are presented in Exhibits 3 to 5.

## Exhibit 3 - Mass Flux in Soil for Soil to Air Pathway

$$D_a = M \times TMP_s + B \qquad \text{Eq. 1}$$

$$D_{es} = D_a \times (P_a)^{10/3} / P_t^2 + D_w + 1/H' \text{ x } (P_w)^{10/3} / P_t^2 \qquad \text{Eq. 2}$$

$$M_s = D_{es} \times A_{con} \times (C_{sg} - C_{sgs}) / L_s \qquad \text{Eq. 3}$$

| Parameter | Definition (units) | Default |
|---|---|---|
| $C_{sgs}$ | Soil gas conc. directly below floor slab or topsoil layer (mg/m$^3$ or ug/L air) | -- |
| $C_{sg}$ | Soil gas conc. in contamination zone | -- |
| $D_a$ | Diffusion in air (m$^2$/sec) | Chemical-specific |
| $D_w$ | Diffusion in water (m$^2$/sec) | Chemical-specific |
| $P_t$ | Total porosity (unitless) | 0.4 |
| $L_s$ | Initial depth from underside of slab or topsoil layer to top of contamination zone (m) | 3 |
| $M_s$ | Diffusive mass flux in soil (mg/sec) | -- |
| $D_{es}$ | Effective diffusivity in soil (m$^2$/sec) | -- |
| $A_{con}$ | Lateral area of contamination (m$^2$) | 1200 (VPH),<br>1700 (LEPH) |
| M, B | Slope and intercept for estimation of diffusion coef. | Chemical-specific |
| $TMP_s$ | Temperature of soil (deg C) | 15 |
| $P_a$ | Air-filled soil porosity (unitless) | 0.2 |
| $P_w$ | Water-filled soil porosity (unitless) | 0.2 |
| H' | Henry's law constant x 42.3 | Chemical-specific |

## Exhibit 4 - Mass Flux Across Surface Slab or Topsoil Layer

$$D_{ec} = D_a \times (C_a)^{10/3} / C_t^2 \qquad \text{Eq. 1}$$

$$D_{ecc} = D_a \times (CC_a)^{10/3} / CC_t^2 \qquad \text{Eq. 2}$$

$$M_d = D_{ec} \times (A_b - A_c) \times (C_{sgs} - C_{ab}) / T_s + D_{ecc} \times A_c \times (C_{sgs} - C_{ab}) / T_s \qquad \text{Eq. 3}$$

$$L_c = 2 \times A_b / S_c \qquad \text{Eq. 4}$$

$$A_c = L_c \times W_c / 1000 \qquad \text{Eq. 5}$$

$$M_s = M_d \text{ (mass continuity)} \qquad \text{Eq. 6}$$

| Parameter | Definition (units) | Default |
|---|---|---|
| $C_{ab}$ | Background ambient air concentration (ug/m$^3$) | 0 |
| $C_a$ | Air porosity of topsoil layer (unitless) | 0.05 |
| $C_t$ | Total porosity of topsoil layer (unitless) | 0.1 |
| $D_{ec}$ | Effective diffusivity in topsoil layer (m$^2$/sec) | -- |
| $CC_a$ | Air porosity of dust-filled cracks in topsoil layer (unitless) | 0.45 |
| $CC_t$ | Total porosity of dust-filled cracks in topsoil layer (unitless) | 0.5 |
| $D_{ecc}$ | Effective diffusivity in concrete cracks in topsoil layer (m$^2$/sec) | -- |
| $S_c$ | Spacing of cracks (m) | 3 |
| $W_c$ | Average crack width (mm) | 1 |
| $A_c$ | Area of cracks (m$^2$) | -- |
| $L_c$ | Total length of cracks (m) | -- |
| $T_s$ | Thickness of topsoil layer (m) | 0.1 |
| $M_d$ | Diffusive mass flux across topsoil layer (mg/sec) | -- |
| $\beta$ | Soil dry bulk density (kg/L) | 1.6 |
| $A_b$ | Area of topsoil layer (m) | 100 |

**Exhibit 5 - Estimation of Ambient Air Concentrations**

$$Q_f = V \times A_b \times DH \quad \text{Eq. 1}$$

$$M_a = C_{ab} \times Q_f \quad \text{Eq. 2}$$

$$C_{air} = (M_d + M_a) / (Q_f) \quad \text{Eq. 3}$$

| Parameter | Definition (units) | Default |
|---|---|---|
| $Q_f$ | Air flow rate ($m^3$/sec) | -- |
| $M_a$ | Mass flux due to ambient conc (mg/sec) | -- |
| $C_{air}$ | Air conc. (mg/$m^3$ or ug/L) | -- |
| V | Wind Speed (m/s) | 2.6 |
| DH | Diffusion height (m) | 2 |
| $C_{ab}$ | Background ambient air concentration (ms/$m^3$ or µg/L) | 0 |

Steady-state mass transport (i.e., no retardation) through subsurface soil is assumed. For soil with relatively high organic carbon contents, retardation and the time required to reach steady-state conditions can be significant. For example, Batterman et al. (1995) reports toluene retardation factors of 17 to 80 for column tests conducted using loam.

Finally, a simple box dispersion model is used to estimate gas concentrations in outdoor air. The box model assumes that soil gas migrating into outdoor airspace is well mixed.

The soil gas transport and exposure modelling was conducted using EXCEL™ and VISUAL BASIC™ macros.

## 5.0 DEFAULT PARAMETERS FOR ENVIRONMENTAL FATE AND TRANSPORT AND EXPOSURE MODELLING EXPOSURE SCENARIO

The default physical parameters used for environmental fate and transport modelling and the source and rationale for their use is presented in Exhibit 6.

**Exhibit 6 - Default Parameters**

**Organic Carbon Content of Soil** ($f_{oc} = 0.006$): The default $f_{oc}$ selected is the default value used in U.S. EPA RAGS Part B (1991). A value of 0.006 is approximately the mid-point of the range of values (0.001 to 0.01) selected by Alberta Environment for input in the derivation of risk-based criteria for petroleum hydrocarbons (unpublished data provided by CPPI).

**Air-filled Porosity Soil** ($P_a = 0.2$): The default air-filled porosity is a best estimate of the approximate average expected value. Air-filled porosity is highly variable and dependent on soil type and moisture conditions. The air-filled porosity at field capacity can range from less than five percent to over forty percent depending on the soil type.

**Total Porosity Soil** ($P_a = 0.4$): The default porosity is a best estimate based on typical range of values provided by Freeze and Cherry (1979).

**Air-filled and Total Porosity of Topsoil** ($C_a = 0.2$, $C_t = 0.4$)

**Air-filled and Total Porosity Cracks** ($CC_a = 0.2$, $CC_t = 0.4$)

**Thickness of Topsoil Layer** ($T_s = 0.1$ m)

**Average Crack Width and Spacing of Cracks** ($W_c = 1$ mm, $S_c = 3$ m).

**Height** (DH = 2 m ): Default value provided in EPA RAGS Part B (1991).

**Wind Speed** (V = 2.6 m/s): Estimated windspeed at 2 m based on Whitehorse data

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